Supplemental material for *B. Savard and G. Blanquart, Effects of dissipation rate and diffusion rate of the progress variable on local fuel burning rate in premixed turbulent flames*

1. Difference with the flamelet equations of Lodier *et al.* [1]

To simplify the comparison, the velocity correction terms (which include diffusion due to gradients in mixture molecular weight), which were found to be negligible in the present flames (see Fig. 7 in the paper), are neglected from both the present flamelet equations and those of Lodier *et al.* [1]. As done in Lodier *et al.* [1], we introduce the following notation for the norm of the gradient of the progress variable: $|\nabla c| = G_c(c)$. It follows that

$$\chi = 2\alpha G_c^2 \tag{1}$$

and

$$\xi = G_c^2 \frac{\mathrm{d}}{\mathrm{d}c}(\rho\alpha) + \rho\alpha G_c \frac{\mathrm{d}G_c}{\mathrm{d}c} - \rho\alpha\kappa G_c. \tag{2}$$

The differential diffusion-induced convective term in Eq. 9 in the paper can be written as

$$\left[\xi\left(\frac{1}{Le_i} - \frac{1}{Le_c}\right) + \frac{\rho\chi}{2}\frac{\mathrm{d}}{\mathrm{d}c}\left(\frac{1}{Le_i} - \frac{1}{Le_c}\right)\right]\frac{\mathrm{d}Y_i}{\mathrm{d}c} = \left[G_c\frac{\mathrm{d}}{\mathrm{d}c}\left(\rho G_c\left(D_i - D_c\right)\right) - \rho\kappa G_c\left(D_i - D_c\right)\right]\frac{\mathrm{d}Y_i}{\mathrm{d}c} \tag{3}$$

The species flamelet equations (Eq. 9 in the paper) can then be expressed as

$$\left[\dot{\omega}_c + G_c\frac{\mathrm{d}}{\mathrm{d}c}\left(\rho G_c\left(D_c - D_i\right)\right) - \rho\kappa G_c\left(D_c - D_i\right)\right]\frac{\mathrm{d}Y_i}{\mathrm{d}c} - \rho D_i G_c^2\frac{\mathrm{d}^2Y_i}{\mathrm{d}c^2} - \dot{\omega}_i = 0, \tag{4}$$

which is similar to Eq. 10 in Lodier *et al.* [1] with the exception of the curvature term, which is absent in their equation.

2. Effect of discretization on the conditional mean

Considering the case where c and χ are the controlling variables, the volumetric conditional mean is computed as

$$
<\dot{\omega}_F|c,\chi>_V = \sum_{\substack{j=1 \\ c-\Delta c<c_j<c+\Delta c \\ \chi-\Delta\chi<\chi_j<\chi+\Delta\chi}}^{M} \dot{\omega}_{F,j}\mathrm{Vol}_j \times \left(\sum_{\substack{j=1 \\ c-\Delta c<c_j<c+\Delta c \\ \chi-\Delta\chi<\chi_j<\chi+\Delta\chi}}^{M} \mathrm{Vol}_j \right)^{-1}, \tag{5}
$$

where M is the total number of data points (11×128^3 times the number of data files) and the subscript i refers to the value at a given grid point. The other conditional means are computed in a similar fashion.

The dissipation rate χ and the tangential strain rate a_t are computed using the same discrete operators as used to perform the simulations with the NGA solver [2]. The curvature κ is obtained using a least-square method given the field of c [3].

To compute the conditional means, the range of each variable is discretized into bins from the minimum value in the domain to the maximum value. In other words, for a mean conditioned on one variable, N bins are considered (such that $\Delta\psi = (\psi_{\max} - \psi_{\min})/N$); for a mean conditioned on two variables, N^2 bins are considered, etc. Bins of constant size are chosen. The conditional means are therefore affected by the choice of N. The larger the number N, the finer the conditional means, but the fewer data points in each bin (reducing the statistical meaning of the mean). Obviously, the most restrictive case is for the mean conditioned on three variables (number of bins equal to N^3). The values of the prediction error for the optimal estimator of the fuel burning rate given a dependence of c, χ, and ξ (non-unity Le) are given in Table 1 for various values of N. It can be seen that for the fuel burning rate $50 < N < 300$, the prediction error is nearly constant.

Note that the mean in each bin is associated to the value of the controlling variables at the center of this bin to create a table. This table is then looked up for the calculation of the prediction error.

Estimator f	ϵ_f
$<\dot{\omega}_F\|c,\chi,\xi>_V$ 300^3 bins	0.200
$<\dot{\omega}_F\|c,\chi,\xi>_V$ 100^3 bins	0.204
$<\dot{\omega}_F\|c,\chi,\xi>_V$ 50^3 bins	0.208

Table 1
Prediction error (Eq. 13 in the manuscript) using different numbers of bins.

References

[1] G. Lodier, L. Vervisch, V. Moureau, P. Domingo, Composition-space premixed flamelet solution with differential diffusion for in situ flamelet-generated manifolds, Combust. Flame 158 (10) (2011) 2009–2016.

[2] O. Desjardins, G. Blanquart, G. Balarac, H. Pitsch, High order conservative finite difference scheme for variable density low mach number turbulent flows, J. Comput. Phys. 227 (2008) 7125–7159.

[3] E. Marchandise, P. Geuzaine, N. Chevaugeon, J. Remacle, A stabilized finite element method using a discontinuous level set approach for the computation of bubble dynamics, J. Comput. Phys. 225 (2007) 949–974.